

CLASS - B.Sc (Hons) PART - III

PAPER - V

TOPIC - THE IR spectra of HCl.

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Q Comment on the IR spectra of HCl.

Ans Molecules having permanent dipole moment e.g. HCl can show IR spectra which are observed in the far IR region.

For a rigid diatomic molecule, the rotational energy is given by

$$E_J = \frac{h^2}{8\pi^2 I} J(J+1) \text{ Joules}$$

where J = rotational quantum number I = moment of inertia and h = Planck's constant. For successive rotational transition -

$$\Delta E = \frac{h^2}{8\pi^2 I} \times 2$$

$$\text{When } J=0, J(J+1) = 0(0+1) = 0$$

$$\text{When } J=1, J(J+1) = 1(1+1) = 2$$

$$\therefore 2 - 0 = 2$$

$$\text{or } h\Delta\bar{\nu}c = \frac{h^2}{4\pi^2 I}$$

$$\text{or } \Delta\bar{\nu} = \frac{h}{4\pi^2 I c} = \frac{h}{4\pi^2 \mu r^2 c} \text{ cm}^{-1}$$

where μ = reduced mass of the molecule and r = internuclear distance. The rotation spectra consist of a series of almost equally spaced lines. The spacing between the successive lines of the maxima corresponds to $\frac{h}{4\pi^2 \mu r^2 c}$

Q Define the terms infrared active and infrared inactive.

Ans The natural vibrational mode within a molecule will absorb radiant energy provided the natural vibrational frequency of the molecule is the same as the frequency of radiation and

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The concerned vibration produces a change in magnitude and direction of dipole moment of the molecule. If an oscillation of the molecule is made impossible by the symmetry of the molecule, such as homonuclear molecules H_2 , O_2 or the $C=C$ mode in ethylene, no radiation corresponding to this oscillation is absorbed. The vibrational mode is said to be inactive. No dipole moment exists or is created in the symmetrical stretching vibration of CO_2 molecule because the centres of gravity of charges coincide in vibrational position and so the vibration is not active. However, in each case of unsymmetrical stretching vibration, the centres of gravity of charges do not coincide. A dipole moment is produced and absorption characteristic of this mode is absorbed in the IR spectrum. The vibrational mode is said to be active.

There occurs dipole moment changes for three vibrations of water, hence it is active.